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Phonon-assisted tunnelling and its dependence on pressure

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Abstract : First the mechanism of phonon-assisted tunnelling has been investigated. The indirect tunnel current density has been computed after taking the amplitude of the time dependent perturbation as the energy of the lattice vibration. Later the pressure dependence of the phonon-assisted tunnel current has been computed using Payne's expression for the dependence of phonon frequency on pressure. Very good qualitative agreements are obtained between predicted and observed characteristics.

Keywords : Tunnel current density, indirect tunnelling, phonon-assisted tunnelling

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1. Introduction

Phonon-assisted tunnelling which comes under the wider area of indirect tunnelling involves the interaction of electrons with the lattice. In fact the nature of interactions allows one to distinguish between a phonon-assisted tunnelling, an impurity assisted tunnelling and the direct tunnelling.

Lattice vibrations play important role in phonon-assisted tunnelling. The energy of electron phonon interaction depends on the amplitude of lattice vibration. When a shear stress or pressure is applied on tunnel devices the current-voltage characteristics undergo changes. These changes are best demonstrated by plotting the curvature of J-V characteristics as a function of bias [1]. Holonyak *et al* [2] studied the J-V curve of a Ge-tunnel diode at 4 K doped with Ga acceptors and Sb donors on the respective sides. These impurities cause a disturbance in the host lattice and tunnelling occurs *via* phonon emission which supplies the wave number difference between the states. At smaller biases the energy difference between the initial and final states is not sufficient to create a phonon of this wave number. But when the bias is increased, for $qV > 7.8$ meV TA (transverse acoustic) phonon and for $qV > 27.5$ meV, LA (longitudinal acoustic) phonon are emitted which cause a sudden rise in the tunnel current at the corresponding biases (7.8 mV and 27.5 mV respectively).

The indirect component (phonon-assisted) consists of several combinations according to the type of phonons such as TA, LA, LO (longitudinal optical) and TO (transverse optical). The values of their onset vc ,ages provide a measure of the phonon energies responsible for them.

Kane [3] calculated the phonon-assisted indirect component of tunnel current using the expression

$$J = \sum_{i,j} CD_{ij}\left[\,|eV|\rangle\ \hbar\,\omega\right] \exp\left(-\beta\right), \tag{1}$$

where

$$\beta = \lambda\left(E_{ij} \pm \hbar\,\omega\right)^{3/2}\left(m_{ij}^{*}\right)^{1/2} \tag{2}$$

The sum includes all combinations of contributing conduction and valence band extrema, labelled by i,j separated by the energy E_{ij}. Here C includes the electron-phonon coupling strength, which is different for different types of phonons. F is average junction field and λ is a constant. The +ve sign is for p to n (reverse bias) tunnelling and the –ve sign for n to p (forward bias) tunnelling. D involves an integral over the initial and final tunnelling states. The mass m_{ij}^{*} is obtained from the effective mass components of the initial and final states extrema along the tunnelling direction x and is given by

$$m_{ij}^{*} = \frac{1}{m_{ix}} \qquad m_{j} \tag{3}$$

Different workers [4–7] have studied this problem in its various aspects.

A quantitative analysis requires a knowledge of the energy shifts and deformations of the energy bands with stress as well as an accurate expression for the tunnel current. However, the threshold voltages for the onset of various tunnelling channels are obtained by simple physical arguments and their shifts under stress can be directly related to shift of critical band edge points or phonon energies.

Pressure and shear stress cause changes in the energies of phonons. Payne [8] measured the shift of the phonon energies with stress. He plotted the second derivative of the tunnel current against bias voltage for an Sb-dopped Ge tunnel diode at 1.2 K. The sharpness of the peaks allows an accurate determination of the energies of the phonons emitted by the indirect tunnelling process. He has tried to quantify his observations as

$$\frac{d \ln \omega_p}{dp} = K\gamma, \tag{4}$$

where ω_p is the phonon frequency, K is the compressibility and γ is the Gruneisen constant.

Some other workers also [9,10] have studied the pressure coefficients of the phonon-assisted tunnel current. Other aspects of phonon-assisted tunnelling have been studied recently [11–14], by different workers, both experimentally and theoretically.

In the present paper, we have used Roy's theory of indirect tunnelling [15,16]. First an expression for electron-phonon interaction has been obtained based on the binding energy approach in crystals. Indirect tunnel current components have been obtained in an attempt to explore the nature of indirect tunnelling due to phonons. Later Payne's idea of the dependence of phonon energy on pressure has been used to calculate the change in phonon-assisted current under applied pressure.

2. Mechanism of phonon-assisted tunnelling

In indirect tunnelling, an electron loses energy by various processes while it tunnels across a potential barrier. When the energy loss is used up in exciting vibrational modes of the molecules present within the barrier, phonons are excited. These excitations interact with tunnelling electrons and provide additional channels to the current flow giving rise to phonon-assisted tunnelling. One sees kinks in the J-V characteristics. A kink in the J-V curve is noticeable at a threshold voltage V such that $qV = \hbar\omega_p$, where ω_p is the phonon frequency when the Fermi levels on the two sides of a tunnel junction differ by a potential V appropriate for exciting a phonon, the additional channel opens up. Thus the J-V characteristics of a tunnel device observed at low temperatures may yield vibrational spectra of molecules present within the barrier. $\frac{d^2J}{dV^2} - V$ characteristics of the tunnel junctions are generally investigated in these studies because they reveal minute discontinuities more distinctly. In Roy's technique indirect transitions across barriers are supposed to be caused by small time-dependent perturbations induced by the excitation just discussed. The electron potential energy under the influence of such external agents may be expressed as [15].

$$V(x, t) = V_1(x) + V_3 \cos \omega_p t, \tag{5}$$

where $V_1(x)$ denotes the potential energy as represented by the barrier shape and $V_3 \cos\omega_p t$ represents the perturbation induced by the above mentioned external agency. The Hamiltonian of the electron in the barrier region is written as

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x, t) \tag{6}$$

$$= H_0 + H_1(t), \tag{7}$$

where $$H_0 = -\frac{\hbar^2}{2m}\cdot\frac{d^2}{dx^2} + V_1(x). \tag{8}$$

The Schrödinger's equations for the unperturbed and perturbed cases may be written as

$$H_0\psi_0(x,t) = i\hbar\frac{\partial}{\partial t}\{\psi_0(x,t)\}, \tag{9}$$

and $$H\psi(x,t) = i\hbar\frac{\partial}{\partial t}\{\psi(x,t)\}. \tag{10}$$

Eq. (9) can be solved by separating the variables, by writing

$$\psi_0(x,t) = X(x)T(t). \tag{11}$$

The solution for $X(x)$ are

$$\left.\begin{aligned} X_1(x) &= \alpha F(x) \\ \text{and}\quad X_r(x) &= \beta G(x) \end{aligned}\right\}, \tag{12}$$

where $F(x)$ and $G(x)$ can be obtained by the linear combination of the solutions of space part of Schrödinger's equation for given shapes of the barrier. For a rectangular barrier one obtains exponentially decaying and growing wave functions.

The solution for $T(t)$ is obtained as

$$T(t) = \gamma\exp\left|-\frac{iE_1t}{\hbar}\right|. \tag{13}$$

Here α, β, γ are constants. α and β may be obtained by matching the incident wave with $X_1(x)$ and the transmitted wave with $X_r(x)$.

The perturbed wave function is written as

$$\psi(x,t) = b_1(t)X_1(x)\exp(i\omega_1 t) + b_r(t)X_r(x)\exp(-i\omega_r t), \tag{14}$$

$b_1(t)$ and $b_r(t)$ are time-dependent coefficients and ω_1 and ω_r respectively denote the angular frequencies of the two states between which an indirect tunnelling transition is made possible by the perturbing terms.

Substituting (14) in (10) and solving it yields

$$|b_1(t)|^2 = \cos^2\left[\frac{Rt}{2}\right] + \frac{(\Delta\omega)^2}{(\Delta\omega)^2+\Omega_0^2}\sin^2\left[\frac{Rt}{2}\right] \tag{15}$$

and $$|b_r(t)|^2 = \frac{\Omega_0^2}{(\Delta\omega)^2+\Omega_0^2}\sin^2\left[\frac{Rt}{2}\right], \tag{16}$$

where $$R = \sqrt{(\Delta\omega)^2+\Omega_0^2}, \tag{17}$$

$$\Delta\omega = \omega_{1r} - \omega_p, \tag{18}$$

$$\omega_{1r} = \frac{E_1 - E_r}{} \tag{19}$$

$$\Omega_0^2 = \frac{M_{12}M_{21}}{\hbar} \tag{20}$$

$$M_{12} = \frac{S_{lr}R_{lr} - S_{lr}R_{rr}}{R_{lr}R_{rl} - R_{ll}R_{rr}} \tag{21}$$

$$M_{21} = \frac{S_{rl}R_{rl} - S_{rl}R_{ll}}{R_{lr}R_{rl} - R_{ll}R_{rr}} \tag{22}$$

$$R_{\mu\nu} = \int_{x_l}^{x_r} X_\mu^* X_\nu dx, \tag{23}$$

$$S_{\mu\nu} = \int_{x_l}^{x_r} X_\mu^* V_3 X_\nu dx, \tag{24}$$

x_l and x_r are the two boundaries of the potential barrier and μ and ν stand for l and r as required.

The electron probability density may be expressed as

$$P(x,t) = \psi^*(x,t)\,\psi(x,t) \tag{25}$$

which finally yields

$$P(x,t) = |X_1(x)|^2 + \frac{|M_{21}|^2 |X_r(x)|^2}{\hbar^2 R^2} \sin^2(RT \tag{26}$$

The first term of eq. (26) represents the direct tunnelling case and the second term gives the tunnelling probability due to indirect tunnelling.

The indirect tunnelling current-density may now be expressed as

$$J_t = q\int_{x_l}^{x_r} \frac{\partial P(x,t)}{\partial t}\Big| \quad dx = J_{0,t} \quad \sin\phi_t \tag{27}$$

where $$J_{0,t} = \frac{q|M_{21}|^2 R_{rr}\tau}{2\hbar^2} \tag{28}$$

and $$\phi_t = R\tau \tag{29}$$

Here, τ is the tunnelling time. The phase ϕ_t is totally uncertain owing to the continuous incidence of electrons. Hence the net indirect tunnel current

$$dJ_i = J_{0,t}\rho_1(E_1)f_1(E_1)dE_1 \sum_{\phi_t=-\infty} \frac{\sin\varphi_t}{\phi_t}, \tag{30}$$

where ρ_1 is the density of states and f_1 is the Fermi-distribution function on the incident end.

The above summation can be easily converted into integration and we have

$$dJ_t = J_{0t}\rho_1(E_1)f_1(E_1)dE_1 \int^{+\infty} \frac{\sin\phi_t\,\hbar}{\phi_t\,\varepsilon_r\,\tau} d\phi_t, \tag{31}$$

where ε_r is energy difference between consecutive energy levels at the transmitted end. Integrating eq. (31) and substituting

$$\frac{1}{\varepsilon_r} = \rho_r(E_1 - \hbar\omega_p)\left\{1 - f_r(E_1 - \hbar\omega_p)\right\}\Omega_r \tag{32}$$

yields
$$dJ_t = \frac{\pi\hbar\Omega_r}{\tau} J_{0i}\rho_1(E_1)f_1(E_1)\rho_r(E_1 - \hbar\omega_p)\left\{1 - f_r(E_1 - \hbar\omega_p)\right\}dE_1. \tag{33}$$

Here Ω_r is the volume of the electrode at the transmitted end. Taking the difference of tunnelling current density both ways we may write

$$dJ_t = \frac{\pi\hbar\Omega_r}{\tau} J_{0t}\rho_1(E_1)\rho_r(E_1 - \hbar\omega_p)\left[f_1(E_1) - f_r(E_1 - \hbar\omega_p)\right]dE_1. \tag{34}$$

But Karlovsky's approximation [17] yields

$$\left[f_1(E_1) - f_r(E_1 - \hbar\omega_p)\right] = \frac{qV}{4k_0T}, \tag{35}$$

where k_0 is Boltzmann's constant.

Hence
$$dJ_t = \frac{qV}{4k_0T}\frac{\pi\hbar\Omega_r}{\tau} J_{0i}\rho_1(E_1)\rho_r(E_1 - \hbar\omega_p)dE_1. \tag{36}$$

For a tunnel diode, we may write the indirect tunnel current density, after substituting appropriate values of parameters in eq. (36) as [18].

$$J_t = C\int_{\hbar\omega_n}^{\Delta E} E^{3/2}\left(E_1 - \hbar\omega_p\right)^{1/2} dE \tag{37}$$

$$C\left\{\Delta E\left(\Delta E - \hbar\omega_p\right)\right\}^{\frac{1}{2}}\left\{\frac{\Delta E^{2}}{3} - \frac{\Delta E\,\hbar\,\omega_p}{12} \quad \frac{(\hbar\omega_p)^2}{8}\right.$$

$$\frac{(\hbar\omega_p)^3}{8}\ \ln\left\{\frac{\sqrt{\Delta E} + \sqrt{\Delta E - \hbar\omega_p}}{\sqrt{\hbar\omega_p}}\right. \tag{38}$$

where
$$C = \frac{2''\sqrt{2}\pi^6\Omega_r q^2 m^{*5/2}\, V_3^2 V}{\hbar^6 k_0 T.E_g^{3/2}}\ \exp\left\{-KE_g^{1/2}\right\}, \tag{39}$$

$$K = \frac{2\sqrt{2}m^{*1/2}\,W}{} \tag{40}$$

and $$\Delta E = E_1 + E_2 - qV, \tag{41}$$

E_g is the energy band gap, W is the width of the barrier and E_1 and E_2 are the Fermi-level degeneracies on the n- and p-sides of the junction.

The amplitude of the perturbation term V_3 appearing in eq. (5) is an undetermined factor so far. For phonon-assisted tunnelling V_3 may be regarded to be the energy of lattice vibration. Thus we may write

$$V_3 = \frac{1}{2} m\omega_p^2 b^2, \tag{42}$$

where m is the mass of a single atom of the semiconductor, ω_p is the frequency of the excited phonon and b is the amplitude of lattice vibration which may be expressed as [19]

$$b = \frac{a}{2}\left(\frac{k_0 T}{B}\right)^{1/2} \tag{43}$$

Here a is the lattice spacing and B is the binding energy. J_t may be calculated for the different phonon frequencies from eq. (38) in which eqs. (39) and (42) have to be substituted.

3. Effect of stress

It can be seen from eqs. (38) and (39) that for a bias V,

$$J_i = P \cdot V_3^2 \cdot V \tag{44}$$

where P is a constant. From eq. (42) and the relation $qV = \hbar\omega_p$, we have

$$J_i = P' \cdot \omega_p^5 \tag{45}$$

where $$P' = \frac{Pm^2 b^4 \hbar}{4q}$$

Hence, $$\ln J_t = \ln P' + 5 \ln \omega_p \tag{46}$$

Therefore, $$\frac{d(\ln J_t)}{dp} = \frac{5d(\ln \omega_p)}{dp} \tag{47}$$

because P' is independent of pressure.

Using Payne's expression [eq. (4)] we have

$$\frac{d(\ln J_i)}{dp} = 5K\gamma. \tag{48}$$

On integrating eq. (48) and using the boundary condition that

$$J_i = J_i(0)$$

when $p = 0$, we finally obtain the pressure dependent indirect tunnel current density as

$$J_i(p) = J_i(0)e^{5K\gamma_p}. \tag{49}$$

Eq. (4) also leads to an expression showing the pressure dependence of phonon-frequency. It is given by

$$\omega_p(p) = \omega_p(0)e^{K\gamma} \tag{50}$$

The dependence of the threshold voltage for phonon excitation on pressure can be easily shown to be

$$V(p) = V(0)e^{K\gamma} \tag{51}$$

where $\omega_p(0)$ and $V(0)$ are phonon frequency and threshold voltage at zero pressure and $\omega_p(p)$ and $V(p)$ are the same at pressure p.

4. Results and discussion

The total tunnel current density consists of the direct tunnel component as well as the indirect one. But the indirect tunnel current density (J_i's) are excited at different threshold voltages. Hence the total current density at a particular bias was computed by adding the direct tunnel component and various indirect components *i.e.*

$$J = J_d + J_{i_1} + J_{i_2} + J_{i_3} + J_{i_4} \tag{52}$$

J_{i_1}, J_{i_2}, J_{i_3} and J_{i_4} are the indirect tunnel current densities due to the four phonons which are excited at the biases 0.008 V, 0.027 V, 0.031 V and 0.036 V in Ge.

The direct tunnel current density J_d was calculated using the expression [16]

$$J_d = AV(\Delta E)^3. \tag{53}$$

No indirect component was added to J_d before 0.008 V. J_{i_1} was added to J_d from 0.008 V onwards, J_{i_2} was added to $J_d + J_{i_1}$ from 0.027 V onwards, J_{i_3} was added to $J_d + J_{i_1} + J_{i_2}$ from 0.031 V onwards and finally J_{i_4} was added to $J_d + J_{i_1} + J_{i_2} + J_{i_3}$ from 0.036 V onwards.

The current-voltage characteristics were drawn as shown in Figure 1. The onset of the different indirect components may be seen in the form of kinks in the J-V curve at the four threshold biases. The kinks become more prominent when $\frac{d^2J}{dV^2}$ is plotted against bias as shown in Figure 2. The pressure dependent indirect tunnel current densities were computed using eq. (49) at four different pressures 7.0×10^7 N/m^2, 2.7×10^8 N/m^2, 5.4×10^8 N/m^2 and 8.1×10^8 N/m^2. Their corresponding threshold biases were computed using eq. (51). However, $\frac{d^2J}{dV^2}$ was computed only for the third phonon (corresponding to $J_{i_3}(p)$). $\frac{d^2J}{dV^2}$ was plotted against V in the vicinity of the corresponding threshold bias for zero pressure as well as for the four applied pressures as shown in Figure 3. If is found that the $\frac{d^2J}{dV^2}$ peaks shift towards higher biases with increasing pressure. Also the peaks go on diminishing with increasing biases.

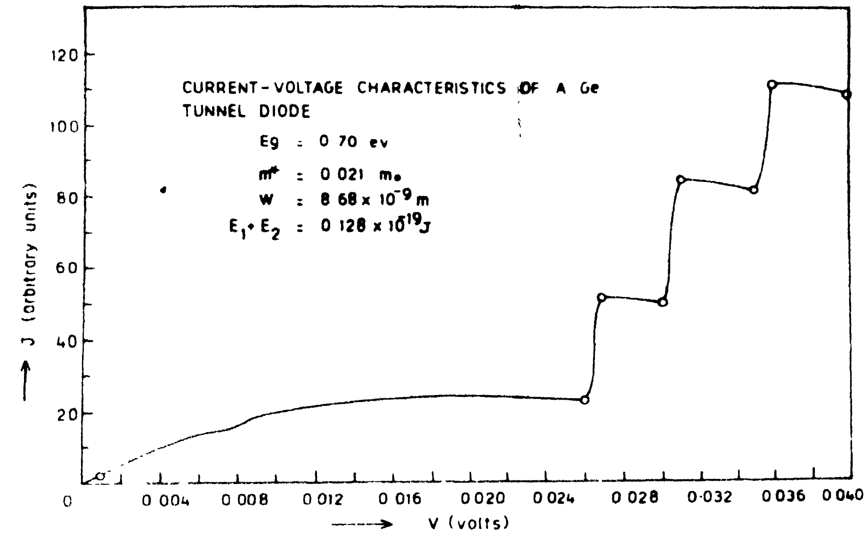

Figure 1. Current-voltage characteristics of a Ge tunnel diode

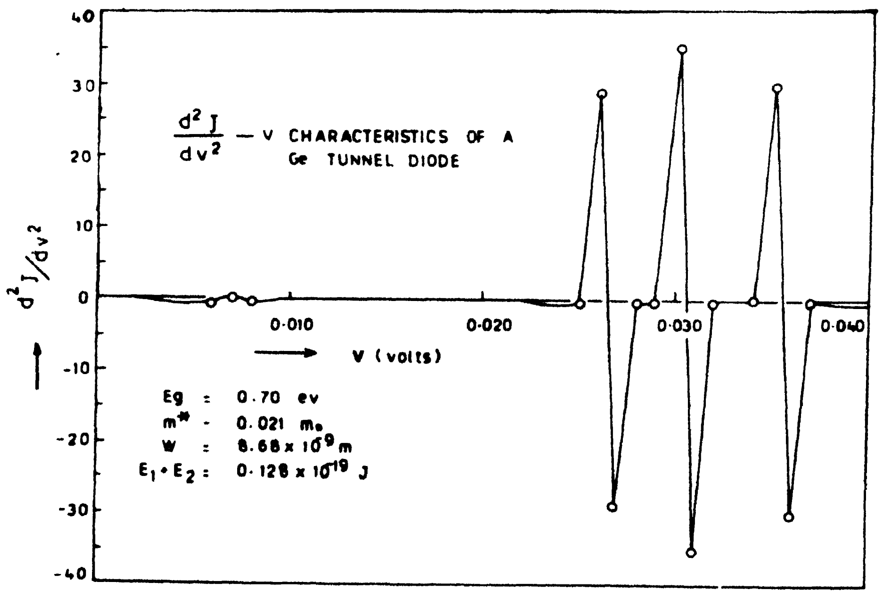

Figure 2. $\frac{d^2J}{dV^2}$ – V characteristics of a Ge tunnel diode

The curve in Figure 1 shows a good qualitative agreement with the work of Fritzsche and Tiemann [6] as the kinks are quite prominent at onset voltages. The curves in Figures 2 and 3 also are in good qualitative agreement with those of Payne [10] as they show all the

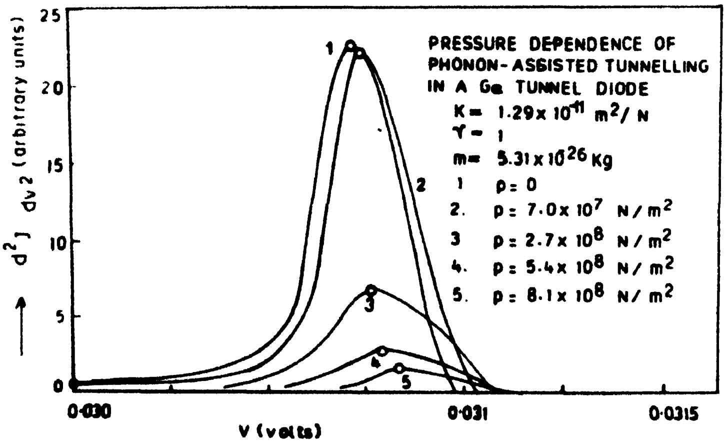

Figure 3. Pressure dependence of phonon-assisted tunnelling in a Ge tunnel diode.

features described in the previous paragraph. Quantitative agreement can also be achieved if exact values of the device parameters are known.

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